Sebastian Thallmair

List of Publications by Year
in descending order

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42 papers	1,599 citations	394421 19 h-index	330143 37 g-index
48 all docs	48 docs citations	48 times ranked	1400 citing authors

#	Article	IF	Citations
1	Protein dynamics and lipid affinity of monomeric, zeaxanthin-binding LHCII in thylakoid membranes. Biophysical Journal, 2022, 121, 396-409.	0.5	9
2	Hypothesis-Driven, Structure-Based Design in Photopharmacology: The Case of eDHFR Inhibitors. Journal of Medicinal Chemistry, 2022, 65, 4798-4817.	6.4	10
3	Perspective: a stirring role for metabolism in cells. Molecular Systems Biology, 2022, 18, e10822.	7.2	12
4	Small ionic radii limit time step in Martini 3 molecular dynamics simulations. Journal of Chemical Physics, 2022, 157, .	3.0	6
5	Running in the Family: Molecular Factors controlling Spin Crossover of Iron(II) Complexes with Schiffâ€base like Ligands. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2021, 647, 905-914.	1.2	6
6	Biaryl sulfonamides as cisoid azosteres for photopharmacology. Chemical Communications, 2021, 57, 4126-4129.	4.1	9
7	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	19.0	557
8	Nonconverged Constraints Cause Artificial Temperature Gradients in Lipid Bilayer Simulations. Journal of Physical Chemistry B, 2021, 125, 9537-9546.	2.6	28
9	Computational Redesign of an Ï‰-Transaminase from Pseudomonas jessenii for Asymmetric Synthesis of Enantiopure Bulky Amines. ACS Catalysis, 2021, 11, 10733-10747.	11.2	28
10	Computational Prediction of Ï‰-Transaminase Specificity by a Combination of Docking and Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2021, 61, 5569-5580.	5.4	17
11	Martini 3 Coarse-Grained Model for Type III Deep Eutectic Solvents: Thermodynamic, Structural, and Extraction Properties. ACS Sustainable Chemistry and Engineering, 2021, 9, 17338-17350.	6.7	20
12	Proteinâ€“ligand binding with the coarse-grained Martini model. Nature Communications, 2020, 11, 3714.	12.8	139
13	Capturing Cholineâ€“Aromatics Cationâ‹¯Ï€ Interactions in the MARTINI Force Field. Journal of Chemical Theory and Computation, 2020, 16, 2550-2560.	5.3	35
14	Unidirectional rotating molecular motors dynamically interact with adsorbed proteins to direct the fate of mesenchymal stem cells. Science Advances, 2020, 6, eaay2756.	10.3	42
15	Molecular dynamics simulations in photosynthesis. Photosynthesis Research, 2020, 144, 273-295.	2.9	50
16	Pitfalls of the Martini Model. Journal of Chemical Theory and Computation, 2019, 15, 5448-5460.	5.3	159
17	Chromophore arrangement in light-harvesting complex II influenced by the protein dynamics on the microsecond time scale. EPJ Web of Conferences, 2019, 205, 09039.	0.3	0
18	Lipid Fingerprints and Cofactor Dynamics of Light-Harvesting Complex II in Different Membranes. Biophysical Journal, 2019, 116, 1446-1455.	0.5	31

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19	An Allosteric Pathway in Copper, Zinc Superoxide Dismutase Unravels the Molecular Mechanism of the G93A Amyotrophic Lateral Sclerosis-Linked Mutation. Journal of Physical Chemistry Letters, 2019, 10, 7740-7744.	4.6	49
20	Ultrafast Reactive Quantum Dynamics Coupled to Classical Solvent Dynamics Using an Ehrenfest Approach. Journal of Physical Chemistry A, 2018, 122, 2849-2857.	2.5	7
21	Cholesterol Flip-Flop Impacts Domain Registration in Plasma Membrane Models. Journal of Physical Chemistry Letters, 2018, 9, 5527-5533.	4.6	36
22	Molecular Dynamcis of Light-Harvesting Complex II Embedded in the Thylakoid Membrane. Biophysical Journal, 2018, 114, 522a.	0.5	0
23	Ultrafast photochemistry with two product channels: Wavepacket motion through two distinct conical intersections. Chemical Physics Letters, 2017, 683, 128-134.	2.6	9
24	Controlling Photorelaxation in Uracil with Shaped Laser Pulses: AÂTheoretical Assessment. Journal of the American Chemical Society, 2017, 139, 5061-5066.	13.7	35
25	Simulating the control of molecular reactions via modulated light fields: from gas phase to solution. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 082001.	1.5	12
26	Design of specially adapted reactive coordinates to economically compute potential and kinetic energy operators including geometry relaxation. Journal of Chemical Physics, 2016, 144, 234104.	3.0	21
27	Two New Methods To Generate Internal Coordinates for Molecular Wave Packet Dynamics in Reduced Dimensions. Journal of Chemical Theory and Computation, 2016, 12, 5698-5708.	5.3	14
28	Molecular features in complex environment: Cooperative team players during excited state bond cleavage. Structural Dynamics, 2016, 3, 043205.	2.3	7
29	Optimal Control Theory for Molecular Reactions in Atomistic Surroundings. , 2016, , .		0
30	How to Control the Ultrafast Dynamics of Uracil with Shaped Laser Pulses: Theoretical Insights. , 2016, , .		0
31	A multi target approach to control chemical reactions in their inhomogeneous solvent environment. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 234003.	1.5	13
32	Quantum Dynamics in an Explicit Solvent Environment: A Photochemical Bond Cleavage Treated with a Combined QD/MD Approach. Journal of Chemical Theory and Computation, 2015, 11, 1987-1995.	5.3	19
33	Quantum Dynamics of a Photochemical Bond Cleavage Influenced by the Solvent Environment: A Dynamic Continuum Approach. Journal of Physical Chemistry Letters, 2014, 5, 3480-3485.	4.6	18
34	The Interplay of Nuclear and Electron Wavepacket Motion in the Control of Molecular Processes: A Theoretical Perspective. Physical Chemistry in Action, 2014, , 213-248.	0.6	3
35	Quantum Dynamics of Molecular Reactions Directed by Explicit Solvent Environment. , 2014, , .		0
36	Ionâ€Pairing of Phosphonium Salts in Solution: Cï£¿Hâ‹…â‹…â‹…Halogen and Cï£¿Hâ‹…â‹…â‹…Ï€ Hydrogen Bonds. Chemistry - A European Journal, 2013, 19, 14612-14630.	3.3	22

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37	Ground and Excited State Surfaces for the Photochemical Bond Cleavage in Phenylmethylphenylphosphonium Ions. Journal of Physical Chemistry A, 2013, 117, 10626-10633.	2.5	6
38	A Comprehensive Microscopic Picture of the Benzhydryl Radical and Cation Photogeneration and Interconversion through Electron Transfer. ChemPhysChem, 2013, 14, 1423-1437.	2.1	22
39	Optimal control theory â€“ closing the gap between theory and experiment. Physical Chemistry Chemical Physics, 2012, 14, 14460.	2.8	63
40	Complete and incomplete spin transitions in 1D chain iron(<scp>ii</scp>) compounds. New Journal of Chemistry, 2011, 35, 691-700.	2.8	49
41	Chemoselective quantum control of carbonyl bonds in Grignard reactions using shaped laser pulses. Physical Chemistry Chemical Physics, 2010, 12, 15780.	2.8	22
42	Strategies towards the purposeful design of long-range ferromagnetic ordering due to spin canting. Polyhedron, 2009, 28, 1796-1801.	2.2	11